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STANFORD UNIVERSITY SCHOOL OF MEDICINE
Department of Genetics

December 16, 1970

Mr. Alan G. Janos
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Kenyon College
P. O. Box 72
Gambier, Ohio   43022

Dear Mr. Janos,

Thank you for your letter of December 11th. I am gratified at your interest in the DENDRAL Program.

Unfortunately, the actual production of the documentation of our system has not kept pace with our expectations or sometimes we have used different routes than were implied in our earlier manuscripts.

Parts IV and V of the NASA report series have not appeared but the entire package will be included in a book I am trying to put together during the next year.

On the same account I have not completed the article originally intended for "Accounts of Chemical Research".

I am sending you the Memo No. 62 that you requested plus some additional writings.

You also request a listing of the source program. Please let me explain why this requires further discussion. A program of this complexity requires continuous attention for its proper maintenance. The program is constantly being patched and revised as well, un-fortunately, as having had to be moved from one computer system to another several times during our experience with it. There is then not one single definitive DENDRAL Program and in order to distribute it we would need a clear mutual understanding of the expectations, facilities, and competence of its recipient.

These problems are enormously magnified by the challenge of moving DENDRAL on to any other and particularly a restricted computer system. Our source program is written in the LISP language. I would be very interested to know if there is any possibility of implementing LISP on the 1130. I suspect not. However, if you do have a LISP capability I will be glad to respond further about the adaptability of our source text.

<u>over</u>

However, do not despair! It may well be both possible and advantageous to re-program the core of the DENDRAL generator so as to run it on a small machine. At worst this might even be programmed in FORTRAN but you will then have many headaches in organizing the dynamic allocation of storage for the assembly of partial structures. With some ingenuity you may be able to trade memory space for time in implementing the algorithm. In LISP-DENDRAL it was very convenient to write the program recursively but this does result in the accumulation of elaborate and voluminous recursion stacks which you would have to avoid.
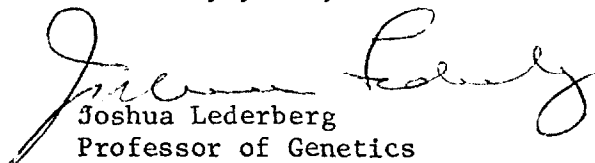
The essential core algorithm is summarized in Table 2 of the first report. I am enclosing a copy marked to focus on the DENDRAL generator for non-cyclic molecules. This is then documented in much greater detail on pages 10 to 15 of Memo. No. 49 which is also on its way to you. The various functions mentioned therein are all written in LISP and will, I fear, almost certainly be jibberish to you. We would ordinarily advocate that a colleague seriously interested in implementing DENDRAL at his own installation spend a month or two working closely with us to be able to work through the entire program. However, I believe you should be able to visualize for yourself how each of the named functions actually operates.

If you could go through the work of parsing through a particular example, like all the isomers of acetic acid, using the general approach outlined here I think you will be able to visualize what would have to be implemented in a computer program.

This Memo describes an earlier version of DENDRAL which has since been superceeded by a table-driven model, which gives much more flexibility in dynamic re-arrangement of the priority of the different "values" listed in Table 2. This is tied in to the heuristics of applying DENDRAL to solving problems of mass-spectrometry, some of which are amplified in great detail in Memo No. 62.

As I indicated I appreciate your interest and that of Professor York and hope that you will find some piece of this program a manageable challenge. Please do not hesitate to call on me further - particularly by phone or in person if this is feasible - if I can be of further assistance.

Sincerely yours,

Joshua Lederberg
Professor of Genetics

JL/rr